Benzeneacetic acid, 4-hydroxy-156-38-7 | DTXSID5059745

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Model Performance

Model	Data	
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Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 8.92e-01

Global applicability domain: Inside

Local applicability domain index: 6.94e-01

Confidence level: 7.35e-01

Nearest Neighbors from the Training Set

Image not found

2-Hydroxyphenylacetic acid

Measured: 0.85 Predicted: 9.03e-01

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Benzeneacetic acid, 4-hydroxy-

Measured: 0.75 Predicted: 8.92e-01

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3-Hydroxyphenylacetic acid

Measured: 0.85 Predicted: 9.01e-01

Image not found

Benzenepropanoic acid, 4-

hydroxy-

Measured: 1.16 Predicted: 1.05

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Methylhydroquinone Measured: 0.91 Predicted: 1.05